Supplemental Material: Macroscopic Thermodynamic Reversibility in Quantum Many-Body Systems

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In this Supplemental Material, we present technically precise statements of Theorem I and Theorem II of the main text. The proof of these theorems will be published elsewhere [62].

I. Precise statement of Theorem I

Theorem S.1. *Let ρ_S be any quantum state on a system S with Hamiltonian H_S, and let $\gamma_S = e^{-\beta H_S} / \operatorname{tr}(e^{-\beta H_S})$. Let $0 \leqslant \epsilon < 1/100$. Suppose that there exists $S \in \mathbb{R}$ and $\Delta > 0$ such that*

$$S^{\epsilon}_{\mathrm{max}}(\rho_S \,\|\, \gamma_S) \leqslant S + \Delta \ ; \qquad \textit{and} \qquad S^{\epsilon}_{\mathrm{min}}(\rho_S \,\|\, \gamma_S) \geqslant S - \Delta \ . \tag{S.1}$$

Then:

(a) There exists a battery system W with energy eigenstates $|0\rangle_W, |w\rangle_W$, a coherence source system C with Hamiltonian H_C and two pure states $|\zeta\rangle_C, |\zeta'\rangle_C$, and a thermal operation $SWC \to SWC$ that maps

$$\rho_S \otimes |w\rangle\langle w|_W \otimes |\zeta\rangle\langle\zeta|_C \to \tilde\rho_{SWC} \ , \tag{S.2}$$

where $\tilde\rho_{SWC} \approx_{\bar\epsilon} \gamma_S \otimes |0\rangle\langle 0|_W \otimes |\zeta'\rangle\langle\zeta'|_C$ and

$$w = \beta^{-1}\Big(-S + 2\Delta + \ln\Big(2m^2\big(\tfrac{36}{\epsilon}\big)^3\Big)\Big) \ ; \tag{S.3a}$$

$$\|H_C\|_\infty \leqslant 3\Delta/\epsilon \ ; \tag{S.3b}$$

$$\bar\epsilon = 13\sqrt{\epsilon} \ , \tag{S.3c}$$

with $\rho \approx_\epsilon \rho'$ denoting proximity in the trace distance, i.e., $\frac{1}{2}\|\rho - \rho'\|_1 \leqslant \epsilon$, and with $m = \lceil \beta(E_{\mathrm{max}} - E_{\mathrm{min}})/\Delta \rceil$ where E_{max} and E_{min} are the maximum and minimum eigenvalues of H_S.

(b) There exists a battery system W' with energy eigenstates $|0\rangle_W, |w'\rangle_{W'}$, a coherence source system C' with Hamiltonian $H_{C'}$ and two pure states $|\xi\rangle_{C'}, |\xi'\rangle_{C'}$,

and a thermal operation $SW'C' \to SW'C'$ that maps

$$\gamma_S \otimes |w'\rangle\langle w'|_{W'} \otimes |\xi\rangle\langle\xi|_{C'} \to \tilde{\rho}'_{SW'C'} \ , \tag{S.4}$$

where $\tilde{\rho}'_{SW'C'} \approx_{\bar{\epsilon}'} \rho_S \otimes |0\rangle\langle 0|_{W'} \otimes |\xi'\rangle\langle\xi'|_{C'}$ *and*

$$w' = \beta^{-1}\Big(S + 2\Delta + \ln\big(\tfrac{2m^3}{\sqrt{\epsilon}}\big) + \tfrac{16}{\Delta\sqrt{\epsilon}}(2\Delta + \ln(2m))^2\Big) \ ; \tag{S.5a}$$

$$\|H_{C'}\|_\infty \leqslant \tfrac{32}{\beta\epsilon^{3/2}\Delta}(2\Delta + \ln(2m))^2 \tag{S.5b}$$

$$\bar{\epsilon}' = 14\sqrt{\epsilon} + m^2 e^{-(2\Delta+\ln(m))} \ , \tag{S.5c}$$

with again $m = \lceil \beta(E_{\max} - E_{\min})/\Delta \rceil$ *where* $E_{\max}$ *and* $E_{\min}$ *are the maximum and minimum eigenvalues of* H_S*.*

The above statement is a slightly specialized version of the full statement in Ref. [62], in which we have chosen $\delta = \beta^{-1}\Delta$ and $q = \epsilon^{-1/2}$.

Furthermore we have expressed all the relative entropies as relative to the Gibbs state $\gamma = e^{-\beta H}/\operatorname{tr}(e^{-\beta H})$, rather than the Gibbs weights operator $e^{-\beta H}$, to simplify the expression of the work cost and yield of transforming to and from the thermal state of S. In a more general case however, one might be interested in transforming between systems with different Hamiltonians. For such situations it is more convenient in Theorem S.1 to consider the transformation of a state ρ_S to and from a trivial thermal state 1 of a trivial one-dimensional system $\mathbb{C}$ with zero Hamiltonian, which serves as a reference thermal state between different systems and Hamiltonians. In this case, the work cost (work yield) is shifted by the constant $-\beta^{-1}\ln\operatorname{tr}(e^{-\beta H_S})$, which is the equilibrium free energy of the thermal state γ_S itself. This can be written more compactly in the relative entropy measure using the unnormalized Gibbs weights, using the property that $S_*(\rho\,\|\,\alpha\sigma) = S_*(\rho\,\|\,\sigma) - \ln(\alpha)$ for all the relative entropy measures considered here. The relative entropy measures in (S.1) are then simply replaced by $S^{\epsilon}_{\min}(\rho\,\|\,e^{-\beta H})$ and $S^{\epsilon}_{\max}(\rho\,\|\,e^{-\beta H})$. (See Ref. [62] for a full statement of the corresponding theorem.)

In the informal statement in the main text, Theorem I, the O-notation refers to a setting where larger and larger system sizes are considered, where the Hamilonian and the quantity S are extensive, $\|H_S\|_\infty \sim n$, $S \sim n$, and where the parameter Δ is at most extensive, $\Delta/S \to 0$, and without loss of generality Δ is chosen to grow at least as $\sqrt{n}$.

II. Precise statement of Theorem II

The asymptotic behavior of the min- and max-relative entropies is characterized by considering the hypothesis testing relative entropy, defined between two states ρ, σ and for any $0 < \eta \leqslant 1$ as [79]

$$S^{\eta}_{\mathrm{H}}(\rho\,\|\,\sigma) = -\log \min_{\substack{0\leqslant Q\leqslant \mathbb{1} \\ \operatorname{tr}(Q\rho)\geqslant\eta}} \eta^{-1}\operatorname{tr}(Q\sigma) \ . \tag{S.6}$$

This relative entropy measure has the property that it is approximately equivalent to the smooth min- and max-relative entropies up to terms that depend only on ϵ (and not the system size) [34, 79]: For $0 < \epsilon < 1/2$, we have

$$S_{\mathrm{H}}^{1-\epsilon^2/6}(\rho \,\|\, \sigma) - \ln\left(\frac{1-\epsilon^2/6}{\epsilon^2/6}\right) \leq S_{\mathrm{min}}^{\epsilon}(\rho \,\|\, \sigma) \leq S_{\mathrm{H}}^{1-\epsilon}(\rho \,\|\, \sigma) - \ln(1-\epsilon) \ ; \tag{S.7a}$$

$$S_{\mathrm{H}}^{2\epsilon}(\rho \,\|\, \sigma) - \ln(2) \leq S_{\mathrm{max}}^{\epsilon}(\rho \,\|\, \sigma) \leq S_{\mathrm{H}}^{\epsilon^2/2}(\rho \,\|\, \sigma) \ . \tag{S.7b}$$

Hence, to show that the min- and max-relative entropies $S_{\mathrm{min}}^{\epsilon}(\rho_n \,\|\, \sigma_n)/n$ and $S_{\mathrm{max}}^{\epsilon}(\rho_n \,\|\, \sigma_n)/n$ asymptotically collapse to the same value, it suffices to show that for any $0 < \eta < 1$, the quantity $S_{\mathrm{H}}^{\eta}(\rho_n \,\|\, \sigma_n)/n$ converges to a value that is independent of η. Indeed, the additional terms in (S.7) vanish because of the $1/n$ prefactor in the $n \to \infty$ limit.

Theorem S.2. *Consider a lattice $\mathbb{Z}^d$ of spatial dimension d and suppose that ρ is translation invariant and ergodic. Consider a translation-invariant Hamiltonian $H = \sum_{z\in\mathbb{Z}^d} h_z$, where h_z is the lattice-translated version of a fixed term h_0 with support on a finite number of sites. For any hypercubic subregion of side length $\ell > 0$, let $n = \ell^d$ and let H_n be the translation-invariant Hamiltonian truncated to contain only those terms supported on the finite region $\{0, \ldots, \ell-1\}^d$ of the lattice. Let $\gamma_n = e^{-\beta H_n}/\operatorname{tr}(e^{-\beta H_n})$ be the Gibbs state associated with the Hamiltonian H_n on the finite subregion. Then, for any $0 < \eta < 1$,*

$$\lim_{\ell\to\infty} \frac{1}{n} S_{\mathrm{H}}^{\eta}(\rho_n \,\|\, \gamma_n) = \lim_{\ell\to\infty} \frac{1}{n} S(\rho_n \,\|\, \gamma_n) =: s(\rho) \ , \tag{S.8}$$

and these limits exist.

Theorem S.2 is a version of Stein's lemma for ergodic states and local Gibbs states. It is proven using techniques that are heavily inspired from Refs. [69, 70, 81–84].

The above theorem may be combined with Theorem S.1 to prove the main result of the paper. For an ergodic state ρ and truncated local Gibbs states γ_n, applying Theorem S.2, we have thanks to (S.7) for $\epsilon > 0$,

$$\lim_{\ell\to\infty} \frac{1}{n} S_{\mathrm{min}}^{\epsilon}(\rho_n \,\|\, \gamma_n) = \lim_{\ell\to\infty} \frac{1}{n} S_{\mathrm{max}}^{\epsilon}(\rho_n \,\|\, \gamma_n) = s(\rho) \ . \tag{S.9}$$

We may define

$$S_{n,\epsilon} = \frac{1}{2}\left[S_{\mathrm{max}}^{\epsilon}(\rho_n \,\|\, \gamma_n) + S_{\mathrm{min}}^{\epsilon}(\rho_n \,\|\, \gamma_n)\right] \ ; \tag{S.10a}$$

$$\Delta_{n,\epsilon} = \frac{1}{2}\left[S_{\mathrm{max}}^{\epsilon}(\rho_n \,\|\, \gamma_n) - S_{\mathrm{min}}^{\epsilon}(\rho_n \,\|\, \gamma_n)\right] \ , \tag{S.10b}$$

which satisfy thanks to (S.9)

$$\frac{1}{n} S_{n,\epsilon} \xrightarrow{n\to\infty} s(\rho) \ ; \qquad\qquad \frac{1}{n} \Delta_{n,\epsilon} \xrightarrow{n\to\infty} 0 \ . \tag{S.11}$$

We may apply Theorem S.1 to each n, ϵ with the given $S_{n,\epsilon}, \Delta_{n,\epsilon}$. This shows that there exist processes to convert ρ_n to γ_n, and vice versa, with corresponding work cost, coherence cost and accuracy given by (S.3) and (S.5). With (S.11), it can be verified that the magnitude of the work cost per copy is equal to $\beta^{-1}S_{n,\epsilon}/n \to \beta^{-1}s(\rho)$ to leading order for both protocols, and the error terms go to zero when taking the limits $n \to \infty$ and then $\epsilon \to 0$. Similarly, the coherence cost per copy as well as the inaccuracy both vanish in these limits. This is Theorem II: The transformations $\rho \to \gamma$ and $\gamma \to \rho$ are possible at a work cost rate (work yield rate) of $\beta^{-1}s(\rho)$ with sublinear requirement of coherence; the accuracy can furthermore be arbitrarily good. (In fact, the two limits $n \to \infty$ and $\epsilon \to 0$ can be taken simultaneously if ϵ goes to zero slowly enough; see details in Ref. [62].)